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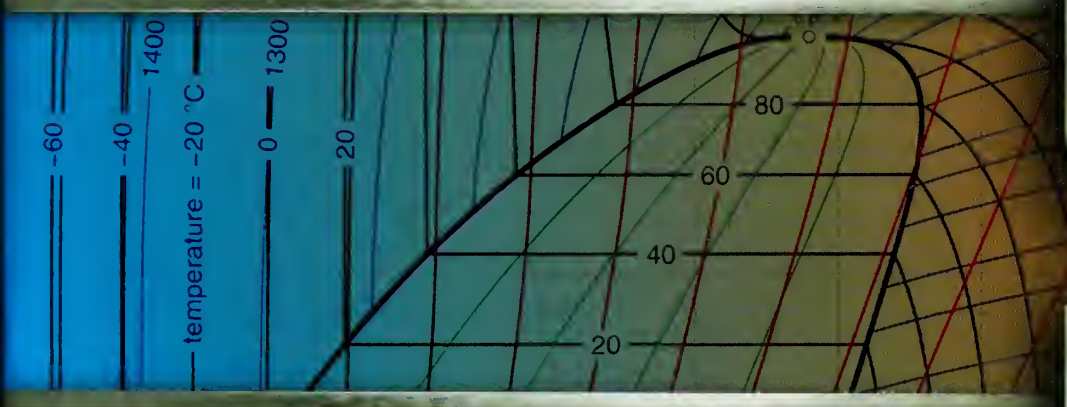
U.S. Department of Commerce
Technology Administration
National Institute of Standards and Technology
Chemical Science and Technology Laboratory

NIST



About the Cover Images, top to bottom:

DNA point mutations in the p53 gene, which are diagnostics for human cancer, are resolved as colored bands through slab gel electrophoresis (see page 9).

Microanalytical compositional mapping of advanced materials and particle populations requires the integration of computer-assisted imaging and spectral deconvolution software (See page 15).

A solid-state titanium-sapphire laser is adjusted for analysis of auto emissions (see page 7).

Physical property relationships for alternative refrigerants, graphically illustrated here for 1,1,1,2-tetrafluoroethane from the NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures database, are needed by industry to design refrigeration systems (see page 11).

A plasma is generated in a Reference Reactor to study etching phenomena and to control plasma cleaning conditions for semiconductor device manufacturing (see page 19).

CHEMICAL SCIENCE AND TECHNOLOGY LABORATORY

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U.S. Department of Commerce
Technology Administration
National Institute of Standards and Technology
Chemical Science and Technology Laboratory

As part of the Commerce Department's Technology Administration, NIST works to promote U.S. economic growth by working with industry to develop and apply technology, measurements, and standards. NIST carries out its mission through a portfolio of four major programs:

- Measurement and Standards Program, consisting of laboratory research and services that are planned and implemented in cooperation with industry and focused on infrastructural technologies, such as measurements, standards, evaluated data, and test methods;
- Advanced Technology Program, which provides cost-shared awards to industry to develop high-risk, enabling technologies with significant economic potential;
- Manufacturing Extension Partnership Program, a network of extension centers and experts providing hands-on technical assistance to smaller manufacturers in adopting new technologies;
- National Quality Program, associated with the Malcolm Baldrige National Quality Award that recognizes continuous improvements in quality management by large manufacturers, service companies, and small businesses.

In fiscal year 1997, NIST is operating on a total budget of more than $700 million with about 3,300 staff members at its sites in Gaithersburg, Maryland (headquarters), and Boulder, Colorado. For further information about NIST, call (301) 975-3058, send e-mail to inquiries@nist.gov, or visit on the World Wide Web at http://www.nist.gov/.

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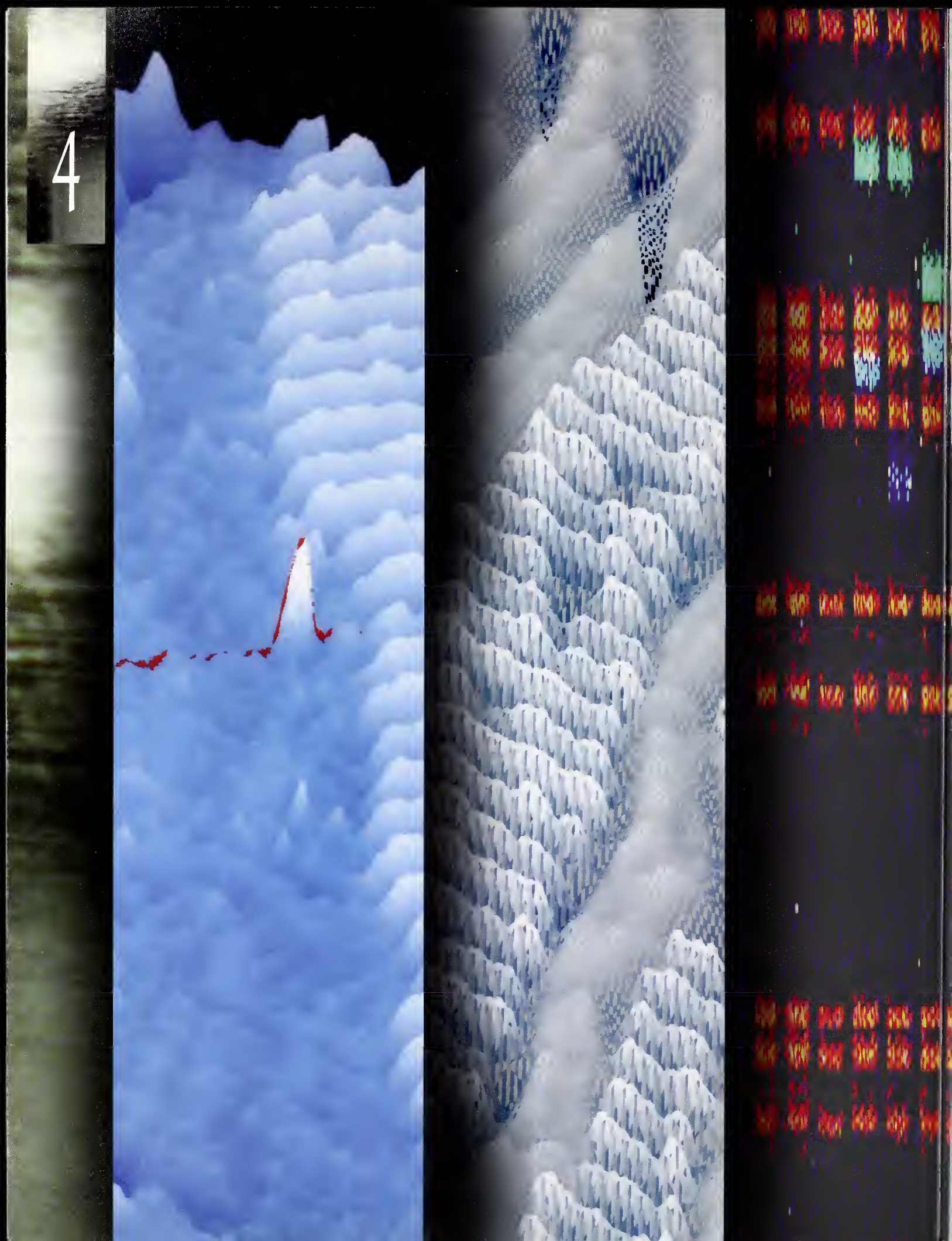
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Message from the Director of the Chemical Science and Technology Laboratory

Since its creation as the National Bureau of Standards in 1901, NIST has been the source of measurements and standards on which industry, commerce, scientific institutions, and all branches of government depend. Reflecting the importance of chemical measurements and standards to our country, the Chemistry Division was one of the very first established by the founders of NIST.

Today, the Chemical Science and Technology Laboratory has the most comprehensive array of chemical, physical, and engineering measurement capabilities of any group working in chemical science and technology.

NIST is the Nation's reference laboratory. CSTL's mission is to perform research in measurement science; develop and maintain measurement methods, standards, and reference data; and develop models for chemical, biomolecular, and physical properties and processes.

An important part of our mission is to anticipate the measurement, standards, and data needs of the U.S. Industry. We assess these needs through interaction with a broad base of customers and through extensive ties to industry, academia, and other government agencies.

Although we place strong emphasis on basic research, our main purpose is to serve you, our customers. We depend on you to help set program priorities, assess the value of our results, and participate in our activities.

I encourage you to learn more about our programs by reading this brochure, and then to join with us in developing the chemical measurement infrastructure that is so important to our Nation.

Dr. Hratch G. Semerjian
Director, Chemical Science and Technology Laboratory
email: hratch.semerjian@nist.gov
URL Address: http://www.cstl.nist.gov/

CHEMICAL SCIENCE AND

THE UNIQUE MISSION of the National Institute of Standards and Technology is to promote U.S. economic growth by working with industry to develop and apply technology, measurements, data, and standards.

The Chemical Science and Technology Laboratory (CSTL) is part of the NIST Measurement and Standards Program. The mission of CSTL is to provide the *chemical measurement infrastructure* to enhance U.S. industry's productivity and competitiveness; assure equity in trade; and improve public health, safety, and environmental quality. CSTL focuses on infrastructural technologies including measurement standards, chemical and process information, and measurement science.

The vision of CSTL is to be a world-class research laboratory recognized by the Nation as the primary resource for chemical, biomolecular, and chemical engineering measurements, data, models, and reference standards required to enhance U.S. industrial competitiveness in the world market. In order to attain this vision, CSTL activities cut across scientific disciplines and focus on the following goals:

Measurement Standards *(page 8)*

- Establish CSTL as the pinnacle of the national traceability and international comparability structure for measurements in chemistry, chemical engineering and biotechnology, and provide the fundamental basis of the nation's measurement system

Chemical and Process Information *(page 10)*

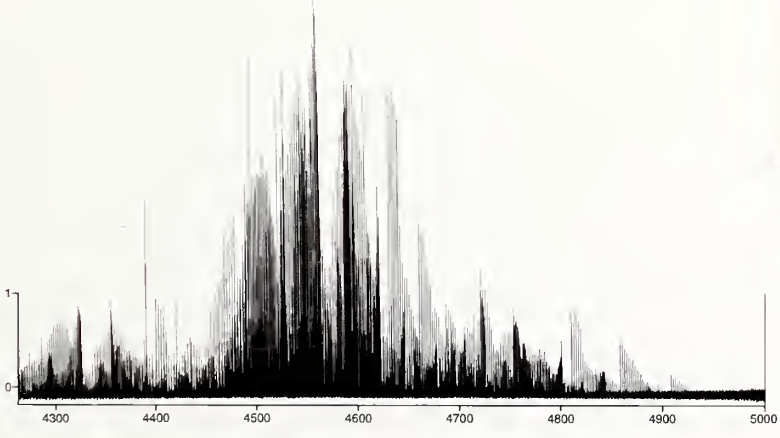
- Assure that U.S. industry has access to accurate and reliable data and predictive models to determine the chemical and physical properties of materials and processes

Measurement Science *(page 14)*

- Anticipate and address next generation measurement needs of the nation, by performing cutting-edge research

TECHNOLOGY LABORATORY

CSTL is working with the American Industry/Government Emissions Research (AIGER) consortium to develop real-time procedures for measuring oxygenated hydrocarbons in auto emissions. This measurement technology is needed to assist in the development of next generation "clean cars" and for monitoring compliance to U.S. EPA and California state regulatory statutes.

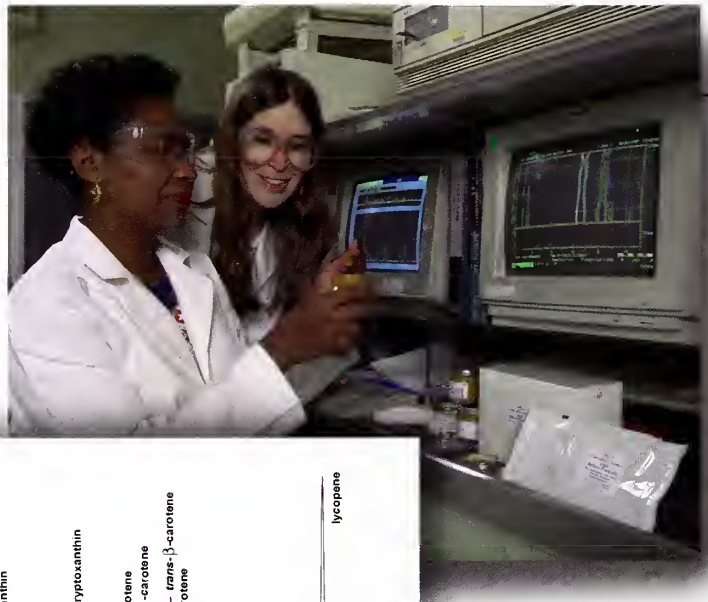


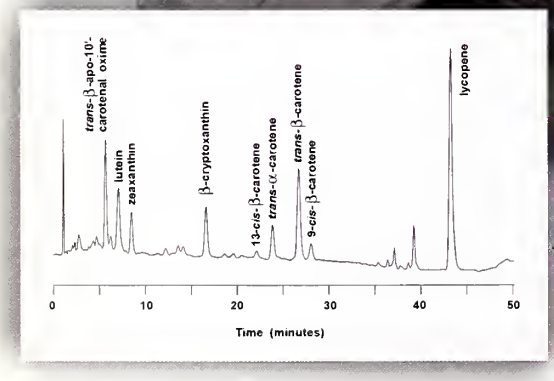
Near-infrared high resolution Fourier-transform spectrum of formaldehyde (taken in collaboration with S. Sharpe and R. Sams at Pacific Northwest National Lab).

MEASUREMENT STANDARDS

A SIGNIFICANT PORTION of U.S. industrial production and international trade is dependent on chemical and physical measurements. Congress in 1901 assigned NIST (then the National Bureau of Standards) the task of maintaining the national measurement system. Key to this system is the development and maintenance of primary and secondary standards, and a national system of measurement traceability to those standards. To meet its measurement responsibilities, CSTL develops and maintains national standards, certifies Standard Reference Materials (SRMs), and offers a wide variety of calibration services (see page 24). We also provide quality assurance services for the health care, environmental, and other industries.

National and international standards influence international trade. Our trading partners around the world are rapidly developing and adopting quality systems that specify and document internationally accepted standards of quality for products, goods, and services. The measurement infrastructure required for U.S. companies to demonstrate conformance with these quality standards has important consequences for the competitiveness of U.S. industry. Physical and chemical measurement standards have significant implications for the market position of U.S. instrumentation and sensor manufacturers. Of greater potential economic significance is the effect that ISO 9000 and ISO 14000 registration, or similar measures, could have on U.S. chemical producers, many of whom are multinational companies. The services and technologies provided by CSTL help U.S. industry meet the broad range of international measurement requirements and compete in global markets.





The Analytical Chemistry Division is working with the Food and Drug Administration and the food industry to produce SRMs that can be used to assist in complying with the Nutrition Labeling and Education Act of 1990. This law requires food processors to provide specific nutrition information on their products' packaging. The accuracy of this information can be improved when food-matrix reference materials are available. Vitamin A values provided on nutrition labels are less accurate than values for other nutrients. NIST is producing SRM 2383, Baby Food Composite, with certified concentrations of vitamin A and ß-carotene (a precursor of vitamin A). A liquid chromatographic (LC) method using a NIST-engineered C_{30} column (chromatogram, inset) and several other LC methods are used to determine carotenoids, including ß-carotene, in SRM 2383.

Mutations of the p53 gene have been implicated in over half of all human cancer cases. Further, breast cancer patients with tumors containing p53 mutations have a poorer survival frequency than those with tumors with normal, or wild type, p53. Detection of p53 mutations in tumors will likely be used to determine the aggressiveness of therapy and provide valuable prognostic information for patients and clinicians. We are using advanced instrumentation to measure the accuracy and sensitivity of two mutation detection assay systems. For these studies, DNA clones containing different mutations have been created by site-directed mutagenesis of the wild type gene. A panel of these clones is being analyzed, and a subset of these clones will be selected as a NIST Standard Reference Material.

CSTL staff provide instruction in the proper techniques for comparison calibration of industrial thermometers and thermocouples. Workshops in precision thermometry are held twice each year. These workshops are excellent ways to transfer new developments and proper measurement techniques to chemical, aerospace, instrument manufacturing, biotechnology industry, power-generating utilities and other government agencies.

Production and characterization of reference materials is a core activity within CSTL. Here, a researcher displays carbon dioxide isotopic Reference Materials distributed worldwide for the intercomparison of ^{13}C and ^{18}O abundance measurements. The proper use of such materials improves interlaboratory measurement reproducibility, important for multilaboratory / multinational studies of environmental systems, international traceability of isotopic data, and improved resolution of isotopic differences in samples for scientific, medical, industrial, and forensic applications.

CHEMICAL AND PROCESS INFORMATION

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CSTL WORKS TO ASSURE that U.S. industry has access to accurate and reliable data, models, and predictive algorithms.

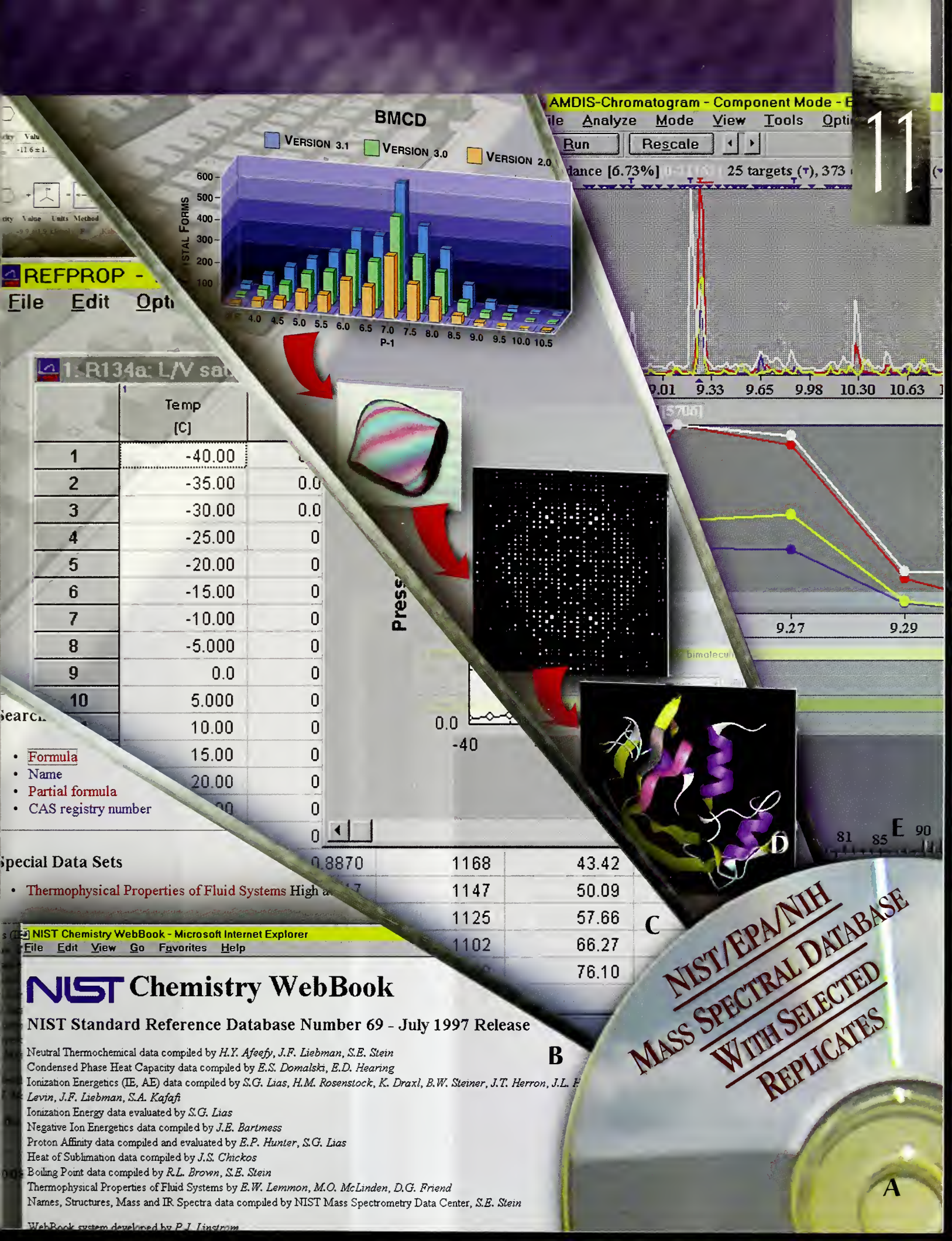
Traditionally, CSTL has been the key source for evaluated data and Standard Reference Data (SRD). Rather than simply being a source for data, we serve as a channel through which customers can access the most reliable data anywhere in the world. This is possible through our evaluated numeric databases, the benchmark measurements we make to fill gaps in databases and to validate models, and the computational approaches we develop for data prediction. The recent addition of the NIST Chemistry WebBook (http://webbook.nist.gov) to the NIST World Wide Web site provides a highly effective tool for data dissemination.

The increasing power of computational tools: Computers are doubling in power every few years, and the importance of computations in scientific and engineering research is growing accordingly. Many industries are now using computational approaches to generate the data needed for accelerated product development and process design and to simulate unit process and plant operation.

A change in emphasis from product development to process improvement: The development of novel and improved processing techniques and new approaches to pollution prevention and control are critical to the economic success of U.S. industry. Technologies that are common to many processes (such as catalysis, oxidation, combustion, and separations) will benefit from CSTL's interdisciplinary approach to their fundamental understanding and application.

CSTL scientists study novel processing techniques such as chemical vapor deposition and plasma processing of semiconductor materials. Our programs also address pollution prevention and pollution control, since the rising costs of waste disposal and environmental regulations may make improved environmental performance of industrial processes a key to economic viability.

Clockwise from lower right: **(A) The NIST/EPA/NIH Mass Spectral Database, available for personal computer use on CD, contains over 75,000 electron-impact mass spectra (over 120,000 spectra in the upcoming version); it is used in the data systems of thousands of mass spectrometers. (B) The NIST Chemistry WebBook is disseminated on the Internet (http://webbook.nist.gov/) and contains thermochemical data for over 5,000 organic and small inorganic compounds, heat of reaction data for over 3,000 reactions, IR spectra for over 5,000 compounds, mass spectra for over 8,000 compounds, ion energetics data for over 14,000 compounds, and thermophysical property data for a select group of industrial fluids. (C) The NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures Database is saving the air conditioning and refrigeration industry millions of dollars as the industry standard for calculating the properties of potential alternative refrigerants. (D) The NIST/NASA/CARB Biological Macromolecule Crystallization Database, also disseminated on the Internet (http://ibm4.carb.nist.gov:4400/bmcd/bmcd.html), contains crystal data and the crystallization conditions for 3,258 crystal entries from 2,297 biological macromolecules for which diffraction quality crystals have been obtained. (E) The Automated Mass Spectral Deconvolution and Identification System, developed in CSTL to support the Defense Special Weapons Agency in their work on the Chemical Weapons Treaty, enables automated chemical weapons inspections with minimal risk of compromising proprietary data.**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1147 50.09
1125 57.66
1102 66.27
76.10
NIST Chemistry WebBook - Microsoft Internet Explorer
File Edit View Go Favorites Help
NIST Chemistry WebBook
NIST Standard Reference Database Number 69 - July 1997 Release
Neutral Thermochemical data compiled by H.Y. Afeefy, J.F. Liebman, S.E. Stein
Condensed Phase Heat Capacity data compiled by E.S. Domalski, E.D. Hearing
Ionization Energetics (IE, AE) data compiled by S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L.
Levin, J.F. Liebman, S.A. Kafafi
Ionization Energy data evaluated by S.G. Lias
Negative Ion Energetics data compiled by J.E. Bartmess
Proton Affinity data compiled and evaluated by E.P. Hunter, S.G. Lias
Heat of Sublimation data compiled by J.S. Chickos
Boiling Point data compiled by R.L. Brown, S.E. Stein
Thermophysical Properties of Fluid Systems by E.W. Lemmon, M.O. McLinden, D.G. Friend
Names, Structures, Mass and IR Spectra data compiled by NIST Mass Spectrometry Data Center, S.E. Stein
WebBook system developed by P.J. Linstrom
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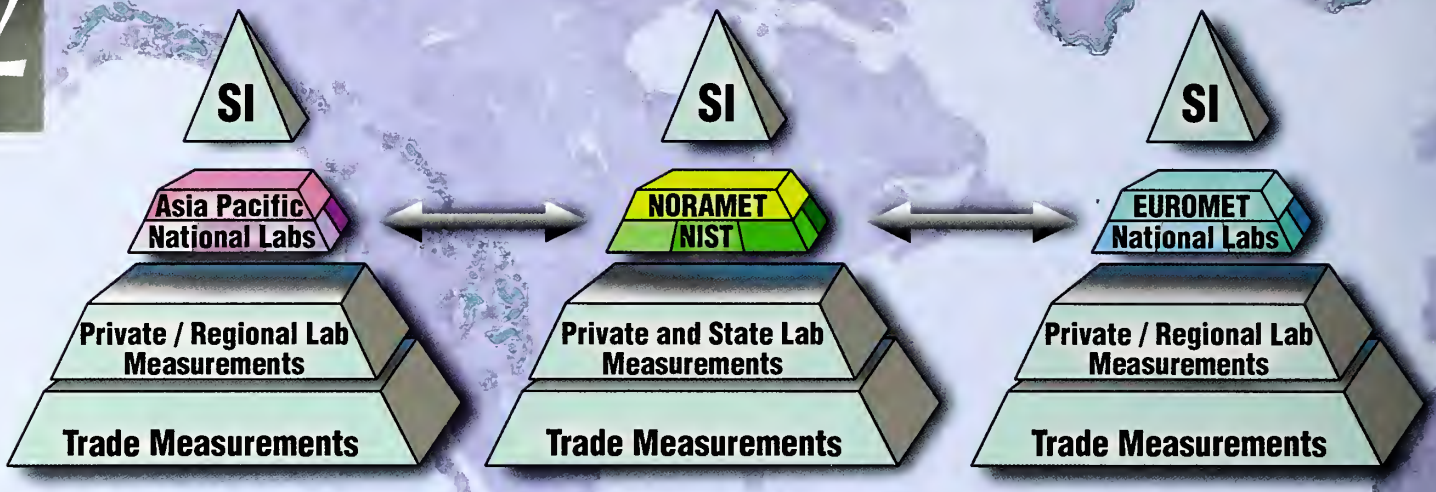
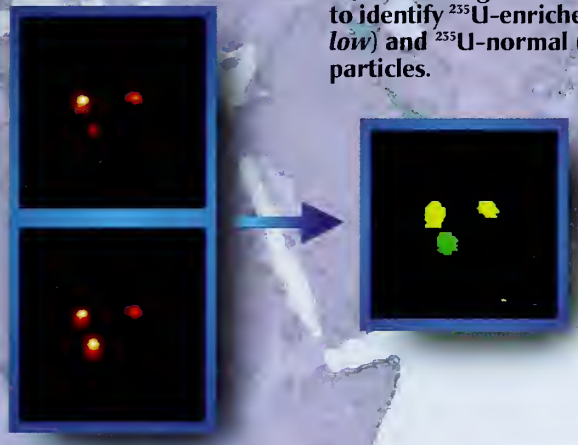
CSTL INTERNATIONAL ACTIVITIES



U.S. trade success in the international marketplace relies in part on overcoming technical measurement barriers and creating a globally accepted measurement and standards infrastructure, depicted above as vertical (national/regional) and horizontal (international) relationships. CSTL is working to harmonize key international standards through bilateral and multilateral comparisons of chemical and physical measurements, technical training exercises, and influential membership in international standards organizations. As a member of the technical committees of the International Committee for Weights and Measures (CIPM), CSTL is responsible for providing the links between chemical and selected physical measurements in the United States and for the International System of Units (SI). Worldwide traceability of chemical and physical measurements is ensured through a highly leveraged system of key Standard Reference Materials, primary methods of chemical analysis, primary physical standards, and calibrations (*e.g.*, temperature, pressure, vacuum, humidity, fluid flow, and air speed). CSTL activities in this international arena positively impact the automotive, environmental, pharmaceutical, petrochemical, agricultural, chemical, and instrument manufacturing industries.

The International Atomic Energy Agency is tasked with global monitoring and verification of the peaceful (non-military) use of civilian nuclear materials. CSTL collaborates in the development of advanced methods and standards for isotopic analysis. In these images, the relative intensities of ^{235}U and ^{236}U SIMS signals are used to identify ^{235}U-enriched (*yellow*) and ^{235}U-normal (*green*) particles.



CSTL staff provide training in the use of their Standard Reference Databases (SRDs) and associated software systems. One such system, coupled to a GC/MS and demonstrated here, is designed specifically for field detection and identification of chemical warfare agents, and will be utilized for verification of compliance to the global Chemical Weapons Treaty.

The NIST Standard Reference Photometer (SRP), developed in cooperation with the EPA, is used worldwide for monitoring ozone levels. Twenty-one SRPs, all built and calibrated by CSTL, are located in the U.S., Canada, Europe, and Australia. The instrument in Bern, Switzerland was recently designated the primary SRP for the Global Atmospheric Watch/World Meteorological Organization (GAW/WMO) project that monitors ground-level ozone in Europe and Africa.

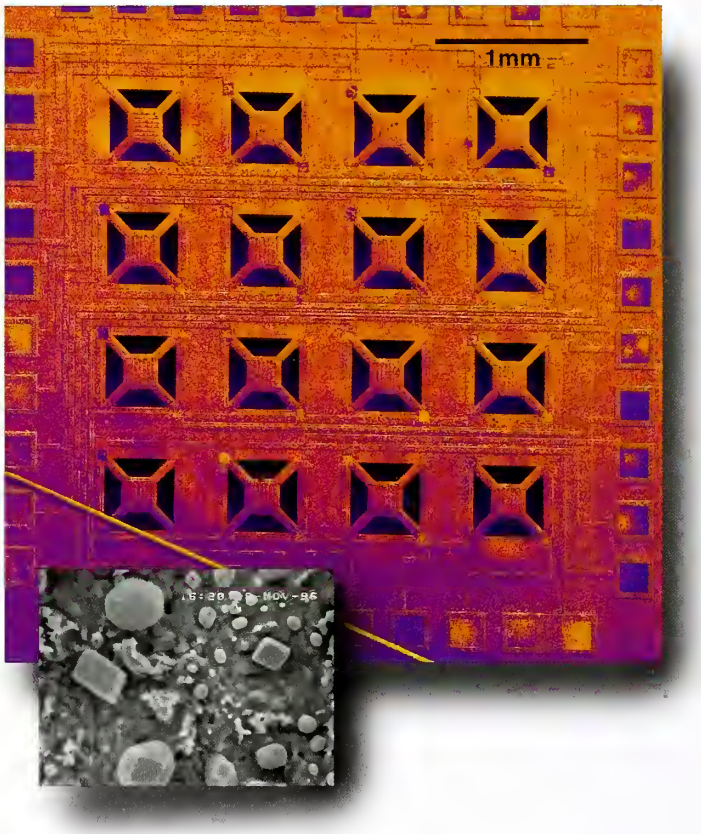
The International Union of Pure and Applied Chemistry (IUPAC) is the recognized world authority on chemical nomenclature, terminology, symbols, units, atomic masses and related topics. NIST involvement with IUPAC is crucial to the establishment of a global standards infrastructure. Staff from several CSTL divisions contribute through their memberships on IUPAC's committees and commissions. Results of their foundational work are frequently published in the IUPAC Journal of Pure and Applied Chemistry.

MEASUREMENT SCIENCE

CSTL MAINTAINS THE TECHNOLOGICAL EDGE required to anticipate the next generation measurement needs of the nation.

One of CSTL's goals is to anticipate the measurement needs of new technologies, so that a measurement infrastructure is available by the time a new technology is implemented. Needs are expanding for accurate, quantitative measurements at ever decreasing detection limits and dimensional scales, in harsher environments, and for a wider range of chemical species. In many cases, these measurements must be performed *in situ* and in real time. These trends derive in part from the need to improve process measurement and control strategies.

Through a strong commitment to basic research, and by leading the advancement of measurement science in critical areas, CSTL is poised to meet these national needs in a timely fashion. Our work involves new concepts in measurement, along with research on the fundamental principles of measurement. For example, CSTL researchers are developing new optical techniques and reference standards for the measurement of very low gas densities. This has important consequences for the semiconductor industry. New measurement techniques are important for a host of industries such as biotechnology, health care, environmental technologies, and the chemical process industry.



CSTL, in collaboration with NIST's Electronics and Electrical Engineering Laboratory, utilizes its expertise in thin-film, solid-state sensing materials, microelectronics fabrication and micro-machining and advanced signal processing to investigate new chemical sensing technologies for gaseous species. Research is focused on response characteristics and mechanisms of semiconducting metal oxide thin films where electrical resistance is changed by molecules attached to the film surface. Metal oxide materials have a moderately chemically-specific electrical response, which can be further tuned for specific chemicals by choosing the set of metal oxides used (e.g., tin, titanium, tungsten, and chromium) and by the addition of various catalytic metals. Addition of small quantities of surface-dispersed, catalytic metals, as shown in the inset, where platinum grains are shown coalescing on the surface of a tin oxide polycrystalline film, further enhances analyte discrimination. The silicon micromachined elements of this 16-element array can be heated individually with small power requirements to temperatures up to 500 °C. This results in additional response variations specific to individual analytes. Arrays such as these are anticipated to be the basis for future multi-species gas sensing technologies. Potential application areas of the technology include chemical, plastics, and semiconductor manufacturing, transportation, and health and safety.

Teamwork in a clean room is frequently necessary for the preparation of particles for chemical and isotopic microanalysis. Here, a CSTL researcher uses an optical microscope to identify particles of interest, and her coworker mounts these particles on a substrate suitable for the subsequent analytical technique (e.g., SIMS, TEM, SEM, AEM)

In collaboration with U.S. industry, a new capability has been developed to determine the thermal and kinetic properties of chemically reacting solids and liquids subject to rapid and controlled heating. This unique device uses laser radiation to achieve the rapidly changing, dynamic high-temperature environments characteristic of 'real world' thermal processes that are not accessible with conventional thermal analysis techniques.

The bender-focuser lens built for the cold neutron prompt gamma activation analysis instrument allows measurements at higher spatial resolution and lower background. The lens consists of 3997 polycapillary lead-glass fibers, each containing 1657 hollow capillary channels of 9.5 μm diameter in a hexagonal arrangement. A portion of the neutron beam is redirected to a focus 95 mm from the exit of the lens and 20 mm below the bottom edge of the incident beam. The lens produces a 0.65mm spot with an intensity gain of about a factor of 25.

CSTL AT A GLANCE

CSTL IS A MULTI-FACETED ORGANIZATION with a broad customer base. We are a national and international resource for chemical and physical measurements and standards, thermochemical, thermophysical and chemical kinetic databases, and predictive models.

We have customers in nearly every industrial sector of the U.S. economy. Certain industries are highly dependent upon CSTL-developed products. For example, over 60 percent of the 4,000 mass spectrometers sold annually by U.S. companies utilize the NIST/EPA/NIH Mass Spectral Database (SRD 1A). Our customers come from both mature and emerging industries, and include the chemical manufacturing, electronics manufacturing, automotive, petroleum refining, measurement and control instrumentation, biotechnology, environmental technologies, and health care industries.

We also serve many federal government agencies, state and local governments, national laboratories, universities, and standards and industrial trade organizations. For example, 80 percent of state forensic laboratories now use the CSTL-certified Standard Reference Materials for DNA profiling, SRM 2390 and SRM 2391.

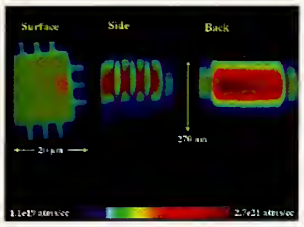
This High Temperature Gas Flow Calibrator (HTGFC) provides U.S. industry with a unique capability to test and evaluate flow meters under realistic usage conditions of variable gas composition, temperature, and flow. Flow measurements of improved accuracy are needed by several industries that utilize combustion processes. The HTGFC differs from other flow meter calibration facilities in its capability to produce gas streams having compositions that range over those normally found in exhaust gas streams from combustion processes. Its maximum operating temperature is 400 °C. CSTL provides this unique capability to U.S. flow meter manufacturers and to flow meter users for test and evaluation of flow metering technologies. Since the availability of the facility in late 1996, interactions between meter manufacturers and NIST researchers resulted in significantly improved metering accuracy. The automotive industry, in collaboration with state and federal environmental regulatory agencies, has taken advantage of this new measurement and standards capability to improve the technological basis for compliance with future clean-air requirements. *Inset:* HTGFC computer-controlled Main Operations Interface, which is used to control gas composition, temperature, and flow rate.

CSTL AT A GLANCE

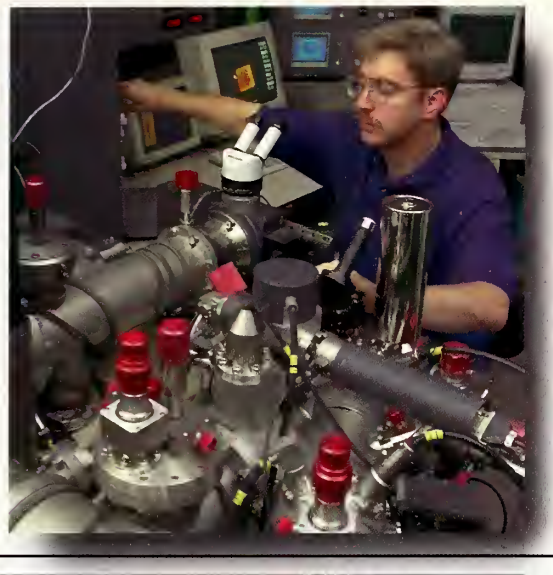
We serve our customers in many ways. CSTL develops and certifies Standard Reference Materials (SRMs) and develops Standard Reference Databases (SRDs). These products are sold to customers directly, as well as through independent distributors. In CSTL, we perform calibrations and analyses, and provide technical expertise to help accredit commercial laboratories through organizations that include the National Voluntary Laboratory Accreditation Program. Customers join consortia, enter into Cooperative Research and Development Agreements (CRADAs), interact through the Advanced Technology Program, license patents on CSTL-developed technologies, and work with us in our laboratories as guest researchers. Over the course of a year, more than 250 visiting researchers work side-by-side with approximately 370 CSTL staff. In some instances, customers contract with us directly for our research and analysis services. Customers also interact with us through measurement assurance programs, conferences and workshops, as well as informal collaborations.

Customer needs shape our program. CSTL staff have extensive ties to industry and also participate widely in national and international committees and professional organizations. These activities take many forms. These include meetings of users of CSTL products and committees of national and international standards organizations, the Council for Chemical Research (CCR), the International Organization for Standardization (ISO), the American Society for Testing and Materials (ASTM), the National Committee for Clinical Laboratory Standards (NCCLS), and the National Conference of Standards Laboratories (NCSL). We also interact with government interagency planning committees, such as the National Science and Technology Council committees on biotechnology and environmental technology and the Calibration Coordination Group (CCG) of the U.S. Department of Defense (DoD). These interactions help us assess industrial and government agency needs and set CSTL program directions.

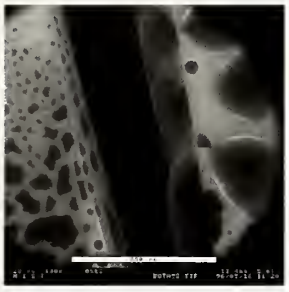
In addition to collaborating with industry, CSTL staff members also collaborate with other technical laboratories within NIST. These efforts provide an additional means for determining and meeting customer needs.



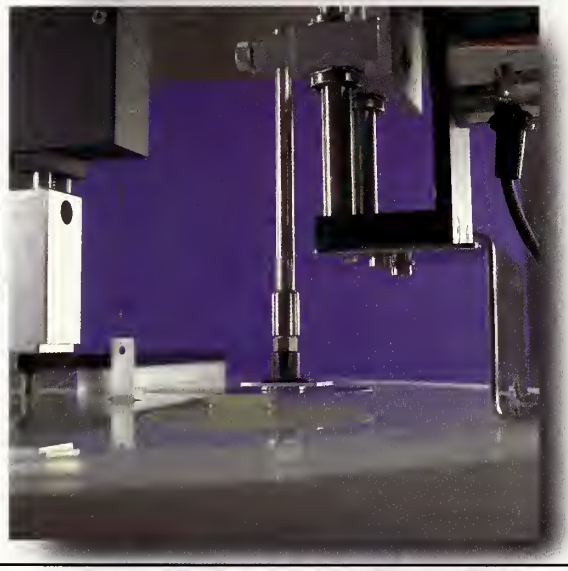
The image shows the 3-dimensional distribution of implanted boron in a semiconductor device.



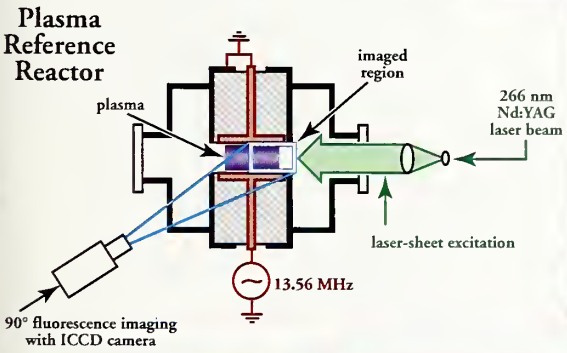
Secondary Ion Mass Spectrometry is used to measure three-dimensional chemical profiles in advanced materials such as semiconductors with a lateral resolution of 0.1 micrometer and a depth resolution of a few nanometers. The chemical compositional map can be used to derive micro-structure/performance property relationships and to improve microfabrication processes.

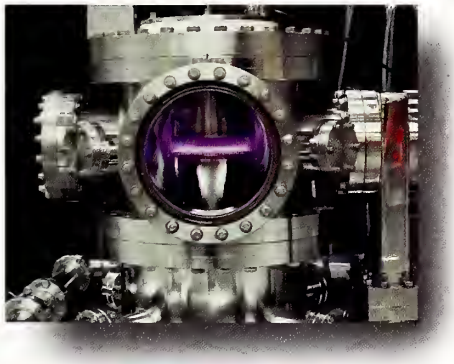


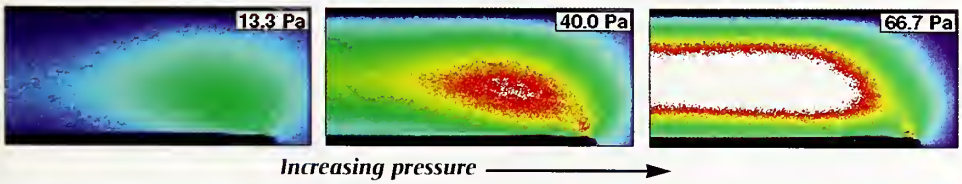
Side-by-side environmental electron micrographs show the differences in water condensation on an alkanethiol-coated Si surface (above right) and a similar surface after exposure to red blood cell (RBC) membranes (above left), indicating that the RBC membrane structure is continuous over the entire surface.



A biomimetic lipid membrane is being formed by transferring a monolayer of phospholipid to a gold surface coated with a self-assembled monolayer of alkanethiol. Using infrared spectroscopy and neutron reflectivity, these samples provide information on membrane and membrane-protein structures. Such information will aid in developing biomimetic materials with application in pharmaceutical screening, sensing, and biocatalysis.





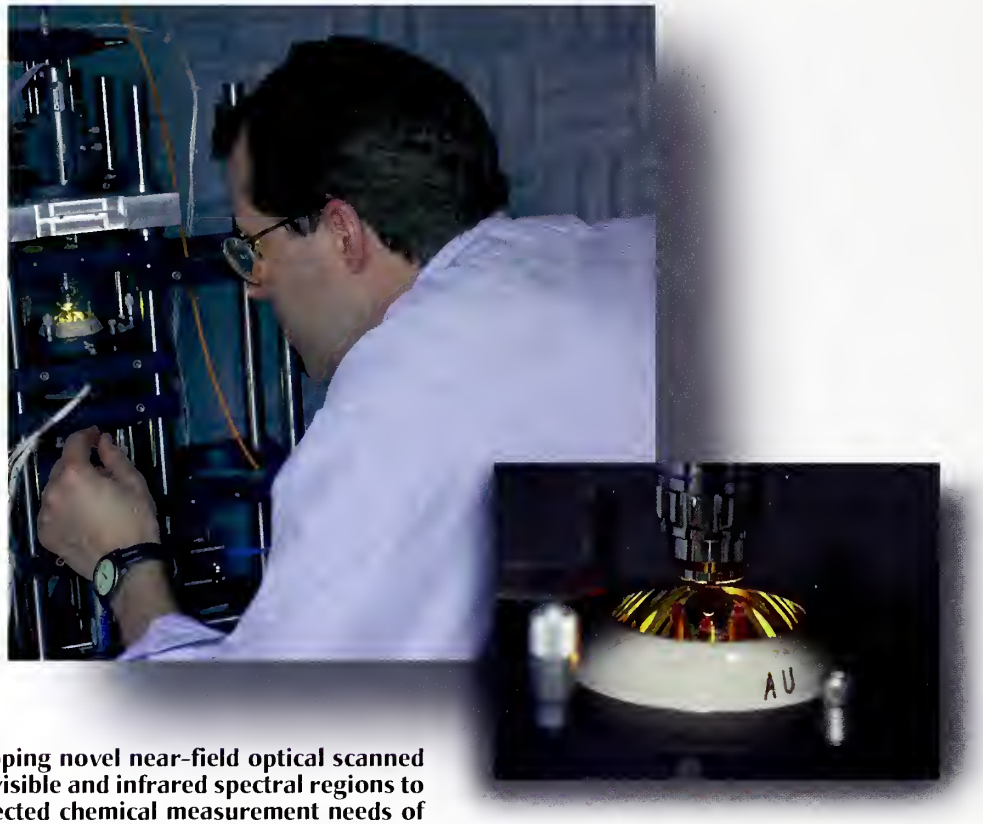


Semiconductor manufacturing requires tight control over plasma processing (etching) and chamber cleanliness. A Radiofrequency (RF) Plasma Reference Reactor is used to facilitate comparison between modeling and experiment in etching and chamber cleaning plasmas. The planar laser-induced fluorescence image of a chemically reactive intermediate (CF_2) in an O_2/CF_4 cleaning plasma demonstrates that spatial density changes with increasing pressure. These results and others dependent on RF current/voltage waveform monitoring can be used to optimize plasma cleaning conditions and reactor operations.

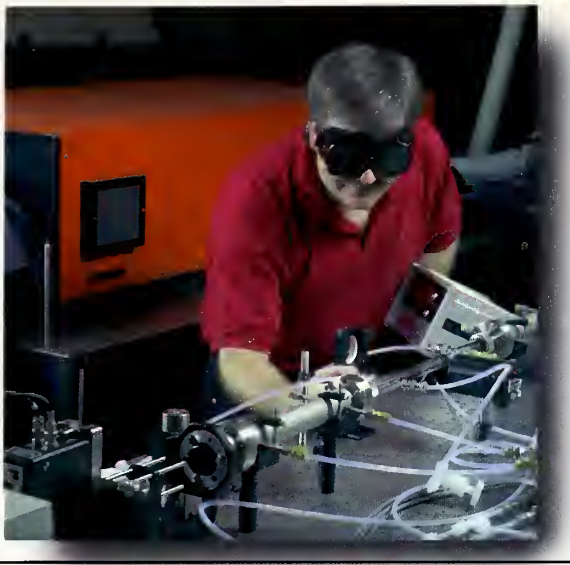
CSTL AT A GLANCE

CSTL maintains a strong basic research program in broad aspects of measurement science that keeps us ready to provide the required measurement, standards, and data capabilities needed to support future technology development. Many of our activities, such as protein crystallography and surface and materials microanalysis, are at the leading edge of science and technology.

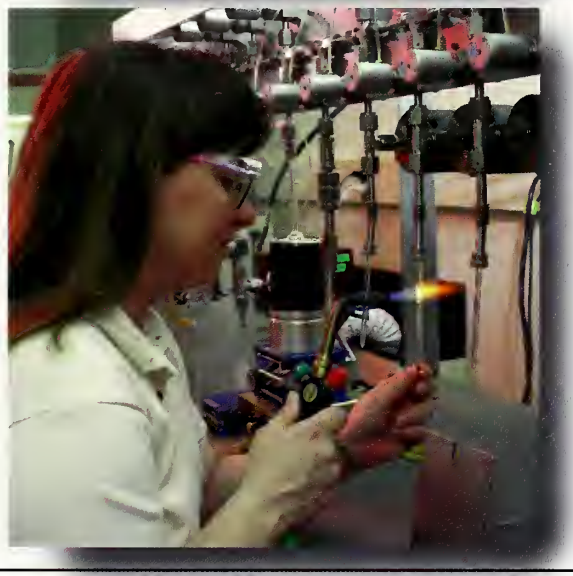
CSTL has a highly acclaimed and multidisciplinary technical staff of chemists, physicists, engineers, biologists, and computer specialists organized in five divisions (see page 22). Many CSTL staff members hold leadership positions in professional societies, standards organizations, and editorial boards of peer-reviewed scientific journals.



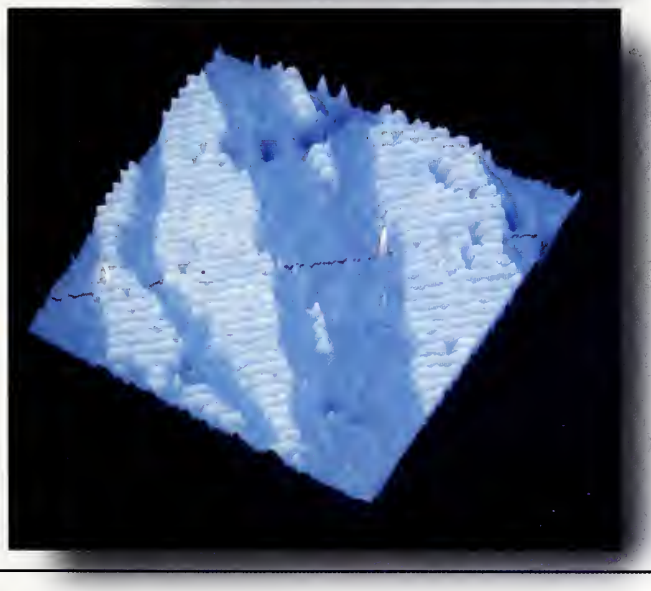
CSTL is developing novel near-field optical scanned probes in the visible and infrared spectral regions to meet the projected chemical measurement needs of industry. The ability to measure chemical bonding changes on the nanometer scale is of critical importance for the characterization of surfaces relevant to heterogeneous catalysis, sensor development, materials science, and biotechnology. These near-field optical techniques are anticipated to provide spatial mapping of chemical-functional-groups on surfaces with 200 nm resolution in the infrared regions. This new form of chemical imaging will provide researchers with an *in situ*, non-destructive probe of site-specific chemistry that will enable engineering improved properties of surfaces.



To improve the quality of kinetic data determined for free-radical reactions, the Physical and Chemical Properties Division has developed an advanced flash photolysis procedure based on laser-excited cavity ring-down techniques.



Highly accurate chemical and isotopic measurement methods on extremely small samples are being developed and applied in environmental studies important to U.S. industry, state and local governments, other federal agencies, and international organizations. Size-limited samples have originated from process residues, chemical speciation, particles from polar ice, aerosols, and atmospheric trace gases. Here, a researcher is preparing a 20 microgram carbon sample for ^{14}C analysis, which will enable the apportionment of the biogenic *vs* anthropogenic components to help identify its origin.



STM topograph of a submonolayer of alkanethiol on Au(111). Striped features are rows of alkanethiol molecules. The red line highlights the additional gold atoms released during adsorption-induced relaxation of the surface during reconstruction. These NIST studies reveal mechanistic pathways of organic monolayer assembly with atomic-level detail, thereby providing fundamental information for commercial developers of organic-monolayer-based biochemical sensors.

THE CSTL DIVISIONS

CSTL's laboratory activities are primarily located at the NIST headquarters site in Gaithersburg, MD. We also have research activities in NIST laboratories in Boulder, CO, and at the Center for Advanced Research in Biotechnology (CARB) in Rockville, MD. CARB is a collaborative effort of NIST, the University of Maryland, and Montgomery County, MD.

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Biotechnology Division

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- *DNA chemistry, sequencing, and profiling*
- *Protein structure determination, properties, and modeling*
- *Biomaterials, biosensors, and bioelectronics*
- *Biocatalysis, bioprocessing measurements, and separations technologies*

Process Measurements Division

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- *Research calibration services and provision of primary standards for temperature, pressure, vacuum, humidity, fluid flow, air speed, liquid density and volume, and gaseous leak-rate measurements*
- *Sensor research:*
  - *Micro-machined gas sensor arrays*
  - *Sensing applications of self-assembled monolayers*
  - *Thin-film thermometry devices*
  - *Pressure, vacuum, and flow sensors*
- *Measurements, models, and data for design and control of semiconductor and materials processing*
- *Engineering models and measurements for control of thermal systems and industrial processes*
- *Multiphase chemical reaction engineering*

Surface and Microanalysis Science Division

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- *Nanoscale chemical characterization*
- *Particle characterization and standards*
- *Electronic and advanced materials characterization*
- *Chemical measurement process*
- *Surface and interface chemistry*
- *Advanced isotope metrology*
- *Molecular scale chemical characterization of organic and biomolecules.*

Physical and Chemical Properties Division

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- *Basic reference data*
- *Data for process and product design*
- *Properties of energy-related fluids*
- *Environmental fates of industrial chemicals*
- *Tools for chemical analysis*
- *Fundamental studies of fluids*
- *Cryogenic technologies*
- *Computational chemistry*
- *Basic measurements and standards*

Analytical Chemistry Division

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- *Chemical measurements research and services in:*
  - *Analytical sensing technologies*
  - *Classical analytical methods*
  - *Gas metrology*
  - *Laboratory automation technology*
  - *Nuclear analytical methods*
  - *Organic analytical methods*
  - *Spectrochemical measurement methods*
- *Tools for achieving international comparability of chemical measurements*
  - *NIST Primary Reference Materials (SRMs)*
  - *NIST Traceable Reference Materials (NTRMs)*
  - *Interlaboratory proficiency testing programs*
  - *International intercomparisons of measurement methods and standards*
- *Critical analytical data and specialty analyses*
  - *Quantitative FTIR database for open path sensing applications*
  - *Aqueous solubility and Henry's Law constants database for environmentally relevant compounds*
  - *Analysis/Chemical characterization of high priority samples*

MAKING CONTACT WITH CSTL

CSTL staff interact with industry, academia, and other government laboratory scientists through a variety of mechanisms including formal and informal collaborations, training workshops, and educational and fellowship programs.

Educational and Fellowship Programs participated in by CSTL

- American Chemical Society Project SEED
- CSTL Graduate Fellowship
- Department of Commerce and Hispanic Association of Colleges and Universities Summer Internship
- National Research Council Postdoctoral Associateship
- NIST Industry Fellowship
- NIST/National Science Foundation (NSF) Faculty Research Program
- NIST Student Career Experience
- NIST Summer Student Temporary Employment
- NIST Summer Student Volunteer
- NIST/University of Colorado Professional Research Experience
- NSF/NIST Graduate Student Research Program

CSTL Assessment of Industrial Needs Workshops

- 2nd International Symposium and Workshop on Biological Environmental Specimen Banking
- 2nd International Symposium of Reversible Associations in Structural and Molecular Biology
- 6th Topical Conference on Quantitative Surface Analysis
- Casting of Aerospace Alloys Workshop
- Catalysis and Biocatalysis Workshop
- Food Reference Materials Needs Workshop
- Measurement and Standards Needs for the Health-Care Community
- Molecular Spectroscopy Data Needs Workshop
- Ninth Annual Workshop on Secondary Ion Mass Spectrometry
- NIST-EPRI Ultrasonic Technology Assessment Workshop
- NIST Traceability in Chemical Spectrophotometry
- PFC Sampling and Measurement Methodologies Technical Working Group
- Sensors, Control, and Robotics Needs of the Process Industries Including the Power Generation Industry
- Symposium on Computational Thermochemistry
- Symposium on the Formation and Control of Combustion-Generated Pollution
- Symposium on Microbeam Analysis in Materials Characterization
- Workshop on Characterization of the Interface/Interphase of Polymer/Substrate Systems
- Workshop on Low-Level Light Standards for Luminometry
- Workshop on Measurement of Sulfur in Superalloys
- Workshop on NIR Glass Wavelength Standards
- Workshop on Thermophysical Properties of Ammonia-Water Mixtures

CSTL Training Workshops

- Calibration and Use of Piston Gauges
- Desk Top Spectrum Analyzer Workshop
- Electron Probe Measurements Workshop
- Fat-Soluble Vitamin and Carotenoid Analysis Tutorial
- NCCLS Workshop on Pb in Blood
- NIST/NCI Micronutrients Measurements Quality Assurance Workshop
- NIST/NOAA Marine Environmental Measurements Quality Assurance Workshop
- Precision Thermometry Workshop
- Raman Measurements Workshop
- Spinning Rotor Gauge Workshop
- Workshop on a Molecular Recognition and Binding Database

Cooperative Research and Development Agreements (CRADAs)

NIST encourages industrial participation in cooperative research with us, and boasts a highly streamlined and individualized CRADA process. Nearly 700 CRADAs have been implemented at NIST since 1988; more than 500 of them were with large or small businesses.

CSTL participated in over 40 such formal collaborative agreements in FY96 alone.

More information on establishing CRADAs with CSTL is available by contacting staff scientists, Division Chiefs, or the NIST Office of Technology Partnerships at (301) 975-3084 or http://ts.nist.gov/ts/htdocs/220.htm.

Internet Access to NIST Information:

http://www.nist.gov/

Internet Access to CSTL Information:

http://www.cstl.nist.gov/

PRODUCTS & SERVICES FROM CSTL

Standard Reference Materials (SRMs)

Ferrous Metals
Nonferrous Metals
High-Purity Materials
Health/Clinical Industrial Hygiene
Gas Standards
Fossil Fuels
Environmental Materials
Food and Agriculture
Geological Materials and Ores
Engine Wear Materials
Ion Activity
Thermodynamic Properties
Optical Properties
Microanalysis

For a complete description, see the *NIST Standard Reference Materials Catalog* available from the NIST SRM sales office, at (301) 975-6776 or http://ts.nist.gov/ts/htdocs/230/232/232.htm

Standard Reference Data (SRD) Products

GRI/NIST Orifice Meter Discharge Coefficient Database (SRD 45)
NIST/ASME Steam Properties Database (SRD 10)
NIST/DIPPR® Properties of Aqueous Solutions Database (SRD 44)
NIST/EPA Gas-Phase Infrared Database (SRD 35)
NIST/EPA/NIH Mass Spectral Database (SRD 1A)
NIST ITS-90 Thermocouple Database (SRD 60)
NIST JANAF Thermochemical Tables Database (SRD 13)
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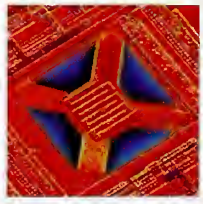
NIST/NASA/CARB Biological Macromolecule Crystallization Database (SRD 21)
NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database (SRD 36)
NIST Chemical Kinetics Database (SRD 17)
NIST Chemical Thermodynamics Database (SRD 2)
NIST Chemistry WebBook (SRD 69)
NIST Estimation of the Thermodynamic Properties for Organic Compounds at 298.15K - Compounds Containing the Elements C, H, N, O, S, and Halogens (SRD 18)
NIST Elastic-Electron-Scattering Cross-Section Database (SRD 64)
NIST Mixture Property Database (SRD 14)
NIST Negative Ion Energetics Database (SRD 19B)
NIST Positive Ion Energetics Database (SRD 19A)
NIST Structures and Properties Database and Estimation Program (SRD 25)
NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures (SRD 23)
NIST Thermophysical Properties of Hydrocarbon Mixtures (SRD 4)
NIST Thermophysical Properties of Pure Fluids (SRD 12)
NIST X-Ray Photoelectron Spectroscopy Database (SRD 20)

For a complete description, see the *NIST Standard Reference Data Products Catalog* available from the NIST Standard Reference Data Program at (301)-975-2208 or http://www.nist.gov/srd/

Calibration Services

Air Speed
Flow Measurements at Cryogenic Temperatures
Fluid Flow
Humidity
Hydrometers
Laboratory Thermometers
Low Pressure, Vacuum, and Leaks
Ozone
Pressure
Resistance Thermometry
Thermocouples, Thermocouple Materials, and Pyrometer Indicators
Volume and Density

For a complete description, see the *NIST Calibration Services User Guide* from the NIST Calibrations Program at (301) 975-2002 or http://ts.nist.gov/ts/htdocs/230/233/233.htm



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Back cover photos clockwise from top left: Aerial view of the NIST headquarters site in Gaithersburg, MD; aerial view of NIST's Boulder, CO, laboratories; Center for Advanced Research in Biotechnology (CARB) in Rockville, MD; artist's rendition (used with permission of Jacobs Engineering Group Inc.) of the Advanced Chemical Sciences Laboratory in Gaithersburg, MD, scheduled for occupancy by CSTL in January 1999.

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August 1997

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